Decision Trees

Nipun Batra and teaching staff

July 21, 2025

IIT Gandhinagar

Discrete Input Discrete Output

The need for interpretability

How to maintain trust in AI

Beyond developing initial trust, however, creators of AI also must work to maintain that trust. Siau and Wang suggest seven ways of "developing continuous trust" beyond the initial phases of product development:

- Usability and reliability. Al "should be designed to operate easily and intuitively,"
 Siau and Wang write. "There should be no unexpected downtime or crashes."
- Collaboration and communication. Al developers want to create systems that
 perform autonomously, without human involvement. Developers must focus on
 creating Al applications that smoothly and easily collaborate and communicate
 with humans.
- Sociability and bonding. Building social activities into AI applications is one way to strengthen trust. A robotic dog that can recognize its owner and show affection is one example, Siau and Wang write.
- Security and privacy protection. Al applications rely on large data sets, so
 ensuring privacy and security will be crucial to establishing trust in the
 applications.
- Interpretability. Just as transparency is instrumental in building initial trust, interpretability – or the ability for a machine to explain its conclusions or actions – will help sustain trust.

Training Data

Day	Outlook	Temp	Humidity	Windy	Play
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
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D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Learning a Complicated Neural Network



Learnt Decision Tree



Medical Diagnosis using Decision Trees



Source: Improving medical decision trees by combining relevant health-care criteria

Leo Brieman



Leo Breiman 1928-2005

Professor of Statistics, <u>UC Berkeley</u>
Verified email at stat.berkeley.edu - <u>Homepage</u>
Data Analysis Statistics Machine Learning



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Optimal Decision Tree

Volume 5, number 1

INFORMATION PROCESSING LETTERS

May 1976

CONSTRUCTING OPTIMAL BINARY DECISION TREES IS NP-COMPLETE*

Laurent HYAFII.

IRIA - Laboria, 78150 Rocquencourt, France

and

Ronald L. RIVEST

Dept. of Electrical Engineering and Computer Science, M.I.T., Cambridge, Massachusetts 02139, USA

Received 7 November 1975, revised version received 26 January 1976

Binary decision trees, computational complexity, NP-complete

Greedy Algorithm

Core idea: At each level, choose an attribute that gives **biggest estimated** performance gain!



 ${\sf Greedy!} {=} {\sf Optimal}$

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• For examples, we have 9 Yes, 5 No

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- Key insight: Problem is "easier" when there is less disagreement

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- Key insight: Problem is "easier" when there is less disagreement
- Need some statistical measure of "disagreement"

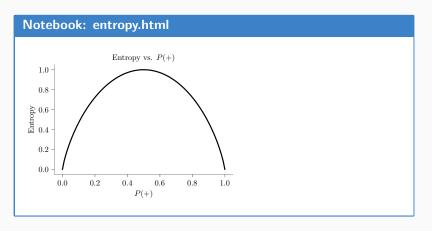
Entropy

Statistical measure to characterize the (im)purity of examples

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$$H(X) = -\sum_{i=1}^k p(x_i) \log_2 p(x_i)$$



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 Can we use Outlook as the root node?

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- Can we use Outlook as the root node?
- When Outlook is overcast, we always Play and thus no "disagreement"

Information Gain

Reduction in entropy by partitioning examples (S) on attribute A

$$\mathsf{Gain}(S,A) \equiv \mathsf{Entropy}(S) - \sum_{v \in \mathsf{Values}(A)} \frac{|S_v|}{|S|} \mathsf{Entropy}(S_v)$$

ID3 (Examples, Target Attribute, Attributes)

• Create a root node for tree

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- Begin

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 - A ← attribute from Attributes which best classifies Examples

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- If all examples are +/-, return root with label =+/-
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 - Root \leftarrow A

- Create a root node for tree
- If all examples are +/-, return root with label =+/-
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 - Root \leftarrow A
 - For each value (v) of A

- Create a root node for tree
- If all examples are +/-, return root with label =+/-
- If attributes = empty, return root with most common value of Target Attribute in Examples
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 - A ← attribute from Attributes which best classifies Examples
 - Root \leftarrow A
 - For each value (v) of A
 - Add new tree branch : A = v

- Create a root node for tree
- If all examples are +/-, return root with label =+/-
- If attributes = empty, return root with most common value of Target Attribute in Examples
- Begin
 - A ← attribute from Attributes which best classifies Examples
 - Root \leftarrow A
 - For each value (v) of A
 - Add new tree branch : A = v
 - Examples_v: subset of examples that A = v

- Create a root node for tree
- If all examples are +/-, return root with label =+/-
- If attributes = empty, return root with most common value of Target Attribute in Examples
- Begin
 - A ← attribute from Attributes which best classifies Examples
 - Root \leftarrow A
 - For each value (v) of A
 - Add new tree branch : A = v
 - ullet Examples_v: subset of examples that A = v
 - If Examples_vis empty: add leaf with label = most common value of Target Attribute

- Create a root node for tree
- If all examples are +/-, return root with label =+/-
- If attributes = empty, return root with most common value of Target Attribute in Examples
- Begin
 - A ← attribute from Attributes which best classifies Examples
 - Root \leftarrow A
 - For each value (v) of A
 - Add new tree branch : A = v
 - ullet Examples_v: subset of examples that A = v
 - If Examples_vis empty: add leaf with label = most common value of Target Attribute
 - Else: ID3 (Examples_v, Target attribute, Attributes A)

Learnt Decision Tree

Root Node (empty)

Training Data

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Entropy calculated

We have 14 examples in S: 5 No, 9 Yes

$$(S) = -p_{\text{No}} \log_2 p_{\text{No}} - p_{\text{Yes}} \log_2 p_{\text{Yes}}$$
$$= -\frac{5}{14} \log_2 \left(\frac{5}{14}\right) - \frac{9}{14} \log_2 \left(\frac{9}{14}\right) = 0.940$$

Outlook	Play
Sunny	No
Sunny	No
Overcast	Yes
Rain	Yes
Rain	Yes
Rain	No
Overcast	Yes
Sunny	No
Sunny	Yes
Rain	Yes
Sunny	Yes
Overcast	Yes
Overcast	Yes
Rain	No

Play

Sunny	No			
Sunny	No			
Sunny	No			
Sunny	Yes			
Sunny	Yes			
We have 2 Yes, 3 No				
$=-\frac{3}{5}\log_2\left(\frac{3}{5}\right)$				
$\frac{2}{5}\log_2\left(\frac{2}{5}\right) = 0.971$				

Outlook

Play

Sunny	No			
Sunny	No			
Sunny	No			
Sunny	Yes			
Sunny	Yes			
We have 2 Yes, 3 No				
$=-\frac{3}{5}\log_2\left(\frac{3}{5}\right)$				
$\frac{2}{5}\log_2\left(\frac{2}{5}\right) = 0.971$				

Outlook

Outlook	Play
Sunny	No
Sunny	No
Sunny	No
Sunny	Yes
Sunny	Yes
A/ I 0 \	/ O NI

We have 2 Yes, 3 No $= -\frac{3}{5} \log_2 \left(\frac{3}{5}\right) - \frac{2}{5} \log_2 \left(\frac{2}{5}\right) = 0.971$

Outlook	Play
Overcast	Yes

We have 4 Yes, 0 No
= 0 (pure subset)

Outlook	Play
Sunny	No
Sunny	No
Sunny	No
Sunny	Yes
Sunny	Yes
A/ I 0 \	/ O NI

We have 2 Yes, 3 No $= -\frac{3}{5} \log_2 \left(\frac{3}{5}\right) - \frac{2}{5} \log_2 \left(\frac{2}{5}\right) = 0.971$

Outlook	Play
Overcast	Yes

We have 4 Yes, 0 No
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Sunny	No
Sunny	No
Sunny	No
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We have 2 Yes, 3 No $= -\frac{3}{5} \log_2 \left(\frac{3}{5}\right) - \frac{2}{5} \log_2 \left(\frac{2}{5}\right) = 0.971$

Outlook	Play
Overcast	Yes

				- 1		
Ve	ha	ave	4	Yes,	0	No
=	0	(рі	ıre	sub	se	t)

Outlook	Play
Rain	Yes
Rain	Yes
Rain	No
Rain	Yes
Rain	No

We have 3 Yes, 2 No
$$= -\frac{3}{5} \log_2 \left(\frac{3}{5}\right) - \frac{2}{5} \log_2 \left(\frac{2}{5}\right) = 0.971$$

Information Gain

$$\mathsf{Gain}(S, \mathsf{Outlook}) = \mathsf{Entropy}(S) - \sum_{v \in \{\mathsf{Rain, Sunny, Overcast}\}} \frac{|S_v|}{|S|} \mathsf{Entropy}(S_v)$$

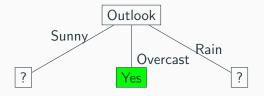
$$(S, \text{Outlook}) = (S) - \frac{5}{14}(S_{\text{Sunny}}) - \frac{4}{14}(S_{\text{Overcast}}) - \frac{5}{14}(S_{\text{Rain}})$$

= $0.940 - \frac{5}{14} \times 0.971 - \frac{4}{14} \times 0 - \frac{5}{14} \times 0.971 = 0.940 - 0.347 - 0 - 0.347 = 0.24$

Information Gain



Learnt Decision Tree



Day	Temp	Humidity	Windy	Play
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• $Gain(S_{Outlook=Sunny}, Temp) = Entropy(2 Yes, 3 No) - (2/5)*Entropy(0 Yes, 2 No) - (2/5)*Entropy(1 Yes, 1 No) - (1/5)*Entropy(1 Yes, 0 No)$

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D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

• $Gain(S_{Outlook=Sunny}, Temp) = Entropy(2 Yes, 3 No) - (2/5)*Entropy(0 Yes, 2 No) - (2/5)*Entropy(1 Yes, 1 No) - (1/5)*Entropy(1 Yes, 0 No)$

Day	Temp	Humidity	Windy	Play
D1	Hot	High	Weak	No
D2	Hot	High	Strong	No
D8	Mild	High	Weak	No
D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

- $Gain(S_{Outlook=Sunny}, Temp) = Entropy(2 Yes, 3 No) (2/5)*Entropy(0 Yes, 2 No) (2/5)*Entropy(1 Yes, 1 No) (1/5)*Entropy(1 Yes, 0 No)$
- Gain($S_{\text{Outlook}=\text{Sunny}}$, Humidity) = Entropy(2 Yes, 3 No) (2/5)*Entropy(2 Yes, 0 No) -(3/5)*Entropy(0 Yes, 3 No) \implies maximum possible for the set

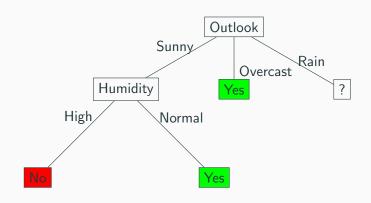
Day	Temp	Humidity	Windy	Play
D1	Hot	High	Weak	No
D2	Hot	High	Strong	No
D8	Mild	High	Weak	No
D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

- $Gain(S_{Outlook=Sunny}, Temp) = Entropy(2 Yes, 3 No) (2/5)*Entropy(0 Yes, 2 No) (2/5)*Entropy(1 Yes, 1 No) (1/5)*Entropy(1 Yes, 0 No)$
- Gain($S_{\text{Outlook}=\text{Sunny}}$, Humidity) = Entropy(2 Yes, 3 No) (2/5)*Entropy(2 Yes, 0 No) -(3/5)*Entropy(0 Yes, 3 No) \implies maximum possible for the set

Day	Temp	Humidity	Windy	Play
D1	Hot	High	Weak	No
D2	Hot	High	Strong	No
D8	Mild	High	Weak	No
D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

- $Gain(S_{Outlook=Sunny}, Temp) = Entropy(2 Yes, 3 No) (2/5)*Entropy(0 Yes, 2 No) (2/5)*Entropy(1 Yes, 1 No) (1/5)*Entropy(1 Yes, 0 No)$
- Gain(S_{Outlook=Sunny}, Humidity) = Entropy(2 Yes, 3 No) (2/5)*Entropy(2 Yes, 0 No) -(3/5)*Entropy(0 Yes, 3 No) ⇒ maximum possible for the set
- $Gain(S_{Outlook=Sunny}, Windy) = Entropy(2 Yes, 3 No) (3/5)*Entropy(1 Yes, 2 No) (2/5)*Entropy(1 Yes, 1 No)$

Learnt Decision Tree



Calling ID3 on (Outlook=Rain)

Day	Temp	Humidity	Windy	Play
D4	Mild	High	Weak	Yes
D5	Cool	Normal	Weak	Yes
D6	Cool	Normal	Strong	No
D10	Mild	Normal	Weak	Yes
D14	Mild	High	Strong	No

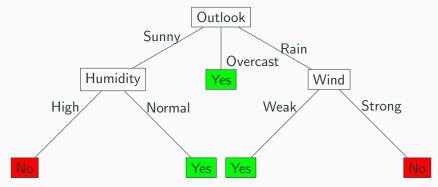
• The attribute Windy gives the highest information gain

Learnt Decision Tree



Prediction for Decision Tree

Just walk down the tree!



Prediction for Decision Tree

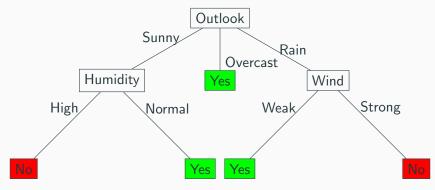
Just walk down the tree!



Prediction for <High Humidity, Strong Wind, Sunny Outlook, Hot Temp> is ?

Prediction for Decision Tree

Just walk down the tree!



Prediction for <High Humidity, Strong Wind, Sunny Outlook, Hot Temp> is ?

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Assuming if you were only allowed depth-1 trees, how would it look for the current dataset?

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What is depth-0 tree (no decision) for the examples? Always predicting Yes

What is depth-1 tree (no decision) for the examples?



Discrete Input, Real Output

Modified Dataset

Day	Outlook	Temp	Humidity	Wind	Minutes Played
D1	Sunny	Hot	High	Weak	20
D2	Sunny	Hot	High	Strong	24
D3	Overcast	Hot	High	Weak	40
D4	Rain	Mild	High	Weak	50
D5	Rain	Cool	Normal	Weak	60
D6	Rain	Cool	Normal	Strong	10
D7	Overcast	Cool	Normal	Strong	4
D8	Sunny	Mild	High	Weak	10
D9	Sunny	Cool	Normal	Weak	60
D10	Rain	Mild	Normal	Weak	40
D11	Sunny	Mild	High	Strong	45
D12	Overcast	Mild	High	Strong	40
D13	Overcast	Hot	Normal	Weak	35
D14	Rain	Mild	High	Strong	20

• Any guesses?

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- Mean Squared Error

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- MSE Reduction = $\mathsf{MSE}(S) \sum_{v} \frac{|S_v|}{|S|} \mathsf{MSE}(S_v)$

Gain by splitting on Wind

Gain by splitting on Wind

Wind	Minutes Played
Weak	20
Strong	24
Weak	40
Weak	50
Weak	60
Strong	10
Strong	4
Weak	10
Weak	60
Weak	40
Strong	45
Strong	40
Weak	35
Strong	20

MSE(S)=311.34

Gain by splitting on Wind

Wind	Minutes Played
Weak	20
Strong	24
Weak	40
Weak	50
Weak	60
Strong	10
Strong	4
Weak	10
Weak	60
Weak	40
Strong	45
Strong	40
Weak	35
Strong	20

$$MSE(S)=311.34$$

Wind	Minutes Player
Weak	20
Weak	40
Weak	50
Weak	60
Weak	10
Weak	60
Weak	40
Weak	35

$$MSE(S_{Wind=Weak}) = 277$$
, $Weight = \frac{8}{14}$

Wind	Minutes Played
Strong	24
Strong	10
Strong	4
Strong	45
Strong	40
Strong	20

$$MSE(S_{Wind=Strong}) = 218$$
, Weight = $\frac{6}{14}$

MSE Reduction Calculation

Correct calculation for Wind split:

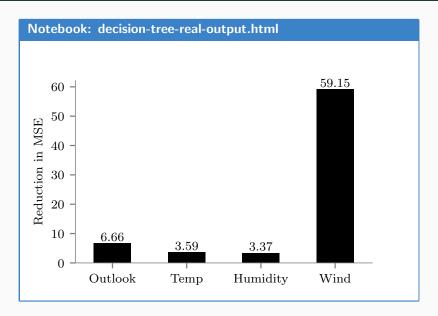
$$MSE Reduction = MSE(S) - Weighted Average MSE$$

$$= 311.34 - \left[\frac{8}{14} \times 277 + \frac{6}{14} \times 218\right] = 311.34 - [158.857 + 93.429] = 311.34$$

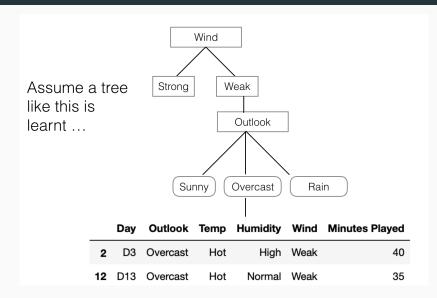
Key insight: MSE Reduction > 0 means the split improves our model!

For regression: Use MSE Reduction, NOT Information Gain!

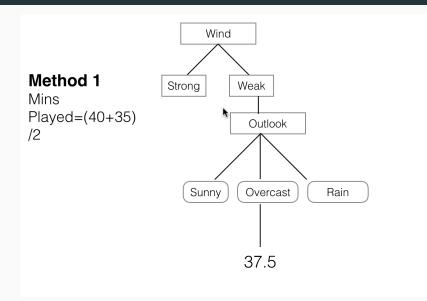
MSE Reduction for Regression Trees



Learnt Tree



Learnt Tree



Real Input Discrete Output

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

• How do you find splits?

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute
- Find potential split points (midpoints).

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute
- Find potential split points (midpoints).
- For the above example, we have 5 potential splits: 44, 54, 66,
 76, 85

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute
- Find potential split points (midpoints).
- For the above example, we have 5 potential splits: 44, 54, 66, 76, 85
- Calculate the weighted impurity for each split

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute
- Find potential split points (midpoints).
- For the above example, we have 5 potential splits: 44, 54, 66, 76, 85
- Calculate the weighted impurity for each split
- Choose the split with the lowest impurity

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

• Consider split at 44

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 44
- LHS has 1 No and 0 Yes; RHS has 3 Yes and 2 No

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 44
- LHS has 1 No and 0 Yes; RHS has 3 Yes and 2 No
- ullet Entropy for LHS = 0, Entropy for RHS = 0.971

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 44
- LHS has 1 No and 0 Yes; RHS has 3 Yes and 2 No
- \bullet Entropy for LHS = 0, Entropy for RHS = 0.971
- Weighted Entropy = 0.971*5/6 = 0.808

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

• Consider split at 54

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 54
- LHS has 2 No and 0 Yes; RHS has 3 Yes and 1 No

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 54
- LHS has 2 No and 0 Yes; RHS has 3 Yes and 1 No
- ullet Entropy for LHS = 0, Entropy for RHS = 0.811

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 54
- LHS has 2 No and 0 Yes; RHS has 3 Yes and 1 No
- \bullet Entropy for LHS = 0, Entropy for RHS = 0.811
- Weighted Entropy = 0.811*4/6 = 0.541

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

• Consider split at 66

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 66
- LHS has 2 No and 1 Yes; RHS has 2 Yes and 1 No

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 66
- LHS has 2 No and 1 Yes; RHS has 2 Yes and 1 No
- ullet Entropy for LHS = 0.918, Entropy for RHS = 0.918

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 66
- LHS has 2 No and 1 Yes; RHS has 2 Yes and 1 No
- ullet Entropy for LHS = 0.918, Entropy for RHS = 0.918
- \bullet Weighted Entropy = 0.918*3/6 + 0.918*3/6 = 0.918

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

• Consider split at 76

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 76
- LHS has 2 No and 2 Yes; RHS has 1 Yes and 1 No

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 76
- LHS has 2 No and 2 Yes; RHS has 1 Yes and 1 No
- ullet Entropy for LHS = 1, Entropy for RHS = 1

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

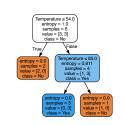
- Consider split at 76
- LHS has 2 No and 2 Yes; RHS has 1 Yes and 1 No
- ullet Entropy for LHS = 1, Entropy for RHS = 1
- $\bullet \ \ \mathsf{Weighted} \ \mathsf{Entropy} = 1 \text{*}4/6 + 1 \text{*}2/6 = 1$

Temperature	PlayTennis
40	No
48	No
60	Yes
72	Yes
80	Yes
90	No
	40 48 60 72 80

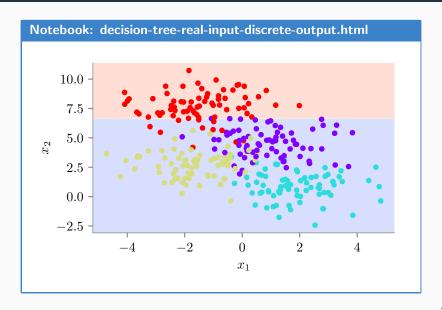
Notebook: decision-tree-real-input-discrete-output.html Temperature ≤ 54.0 entropy = 1.0 samples = 6 value = [3, 3] class = No True \False entropy = 0.0 entropy = 0.811 samples = 2 samples = 4 value = [2, 0] value = [1, 3] class = No class = Yes

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

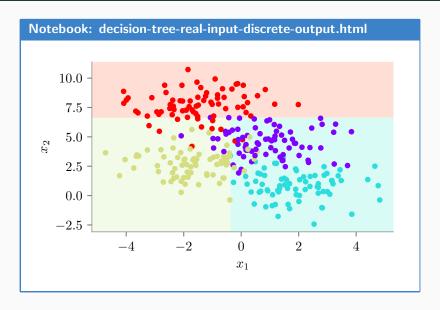
Notebook: decision-tree-real-input-discrete-output.html



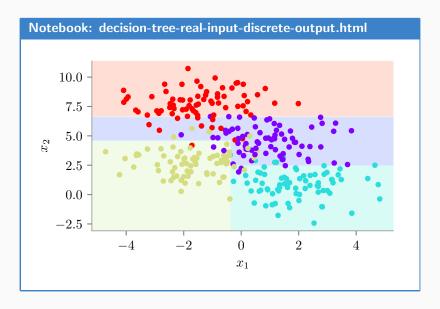
Example (DT of depth 1)



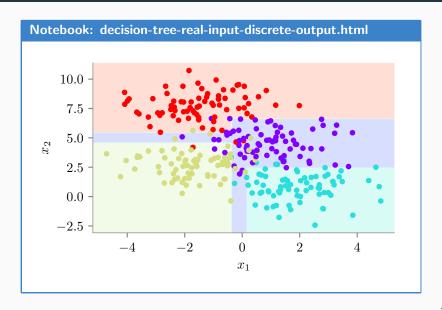
Example (DT of depth 2)



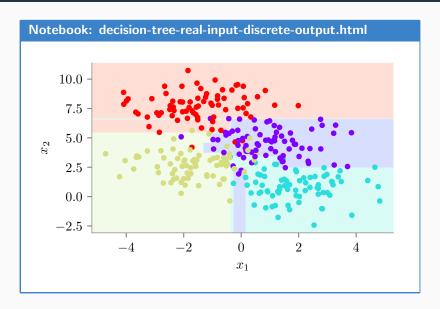
Example (DT of depth 3)



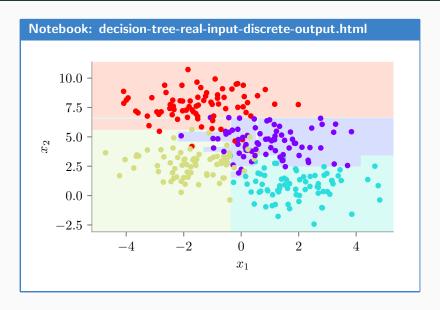
Example (DT of depth 4)



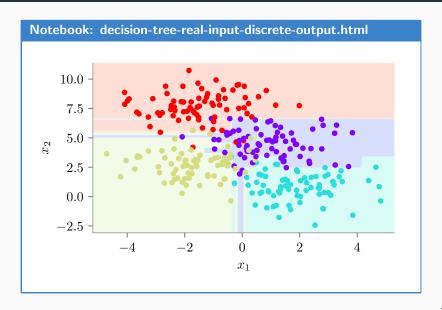
Example (DT of depth 5)



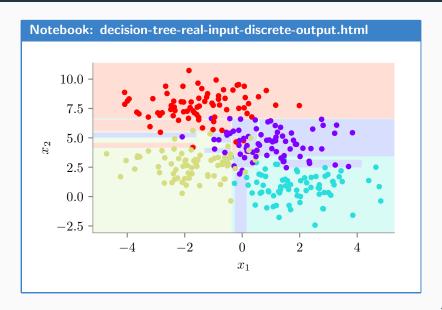
Example (DT of depth 6)



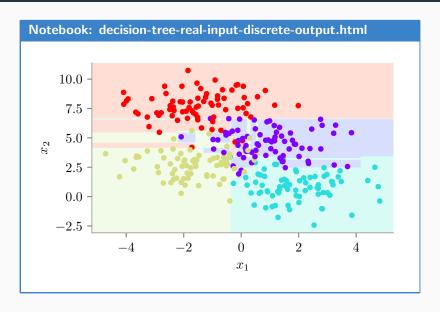
Example (DT of depth 7)



Example (DT of depth 8)

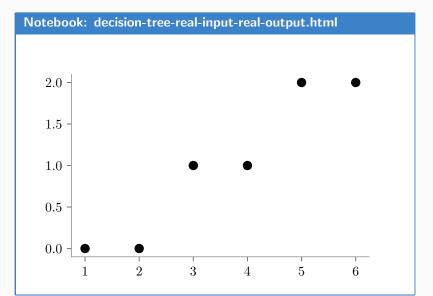


Example (DT of depth 9)

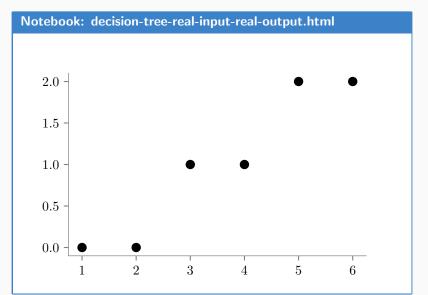


Real Input Real Output

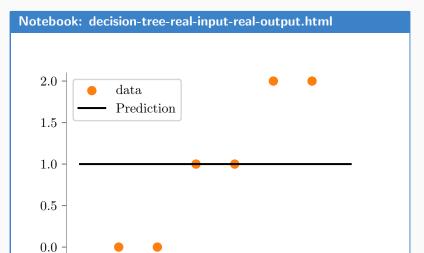
Let us consider the dataset given below



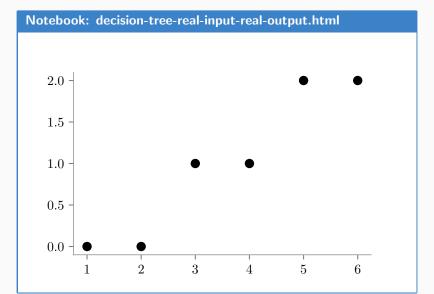
What would be the prediction for decision tree with depth 0?



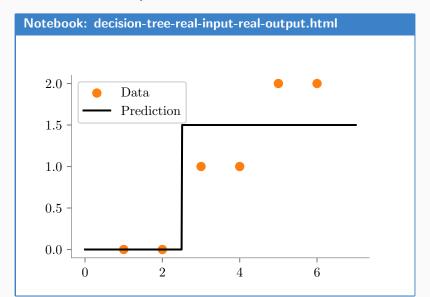
Prediction for decision tree with depth 0. Horizontal dashed line shows the predicted Y value. It is the average of Y values of all datapoints.



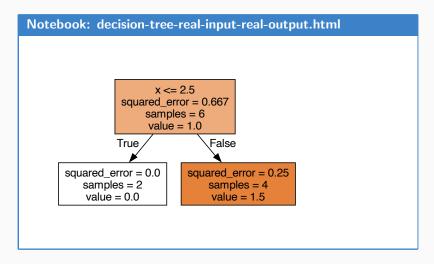
What would be the decision tree with depth 1?



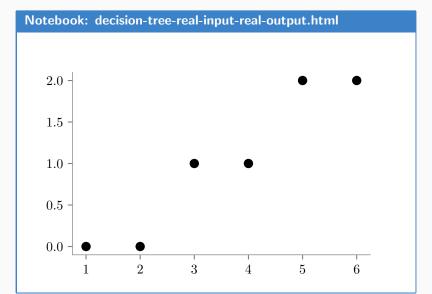
Decision tree with depth 1



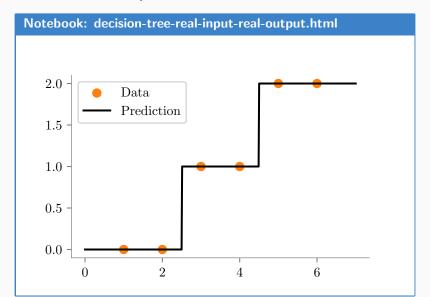
The Decision Boundary



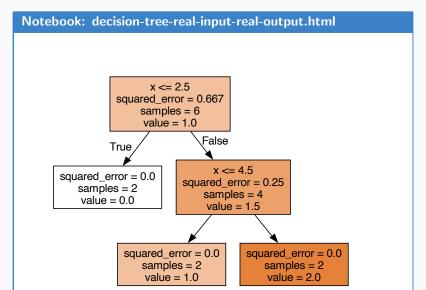
What would be the decision tree with depth 2?



Decision tree with depth 1



The Decision Boundary



Objective Function for Regression Trees

Feature is denoted by X and target by Y.

Let the split be at X = s.

Define regions: $R_1 = \{x : x \le s\}$ and $R_2 = \{x : x > s\}$.

Objective Function for Regression Trees

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Let the split be at X = s.

Define regions: $R_1 = \{x : x \le s\}$ and $R_2 = \{x : x > s\}$.

For each region, compute the mean prediction:

$$c_1 = \frac{1}{|R_1|} \sum_{x_i \in R_1} y_i$$

$$c_2 = \frac{1}{|R_2|} \sum_{x_i \in R_2} y_i$$

Objective Function for Regression Trees

Feature is denoted by X and target by Y.

Let the split be at X = s.

Define regions: $R_1 = \{x : x \le s\}$ and $R_2 = \{x : x > s\}$.

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$$c_1 = \frac{1}{|R_1|} \sum_{x_i \in R_1} y_i$$

$$c_2 = \frac{1}{|R_2|} \sum_{x_i \in R_2} y_i$$

The loss function is:

Loss(s) =
$$\sum_{x_i \in R_1} (y_i - c_1)^2 + \sum_{x_i \in R_2} (y_i - c_2)^2$$

Objective Function for Regression Trees

Feature is denoted by X and target by Y.

Let the split be at X = s.

Define regions: $R_1 = \{x : x \le s\}$ and $R_2 = \{x : x > s\}$.

For each region, compute the mean prediction:

$$c_1 = \frac{1}{|R_1|} \sum_{x_i \in R_1} y_i$$

$$c_2 = \frac{1}{|R_2|} \sum_{x_i \in R_2} y_i$$

The loss function is:

Loss(s) =
$$\sum_{x_i \in R_1} (y_i - c_1)^2 + \sum_{x_i \in R_2} (y_i - c_2)^2$$

Our objective is to find the optimal split:

Algorithm: Finding the Optimal Split

1. Sort all data points (x_i, y_i) in increasing order of x_i .

Algorithm: Finding the Optimal Split

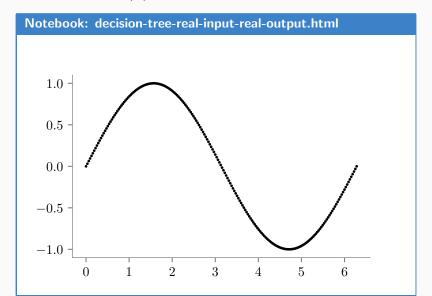
- 1. Sort all data points (x_i, y_i) in increasing order of x_i .
- 2. Evaluate the loss function for all candidate splits:

$$s = \frac{x_i + x_{i+1}}{2}$$
 for $i = 1, 2, ..., n-1$

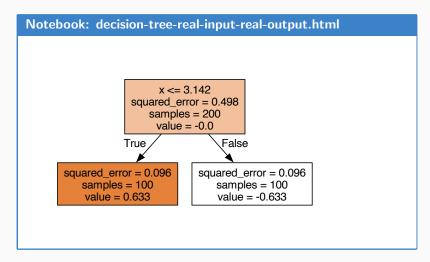
Algorithm: Finding the Optimal Split

Draw a regression tree for Y = $\sin(X)$, $0 \le X \le 2\pi$

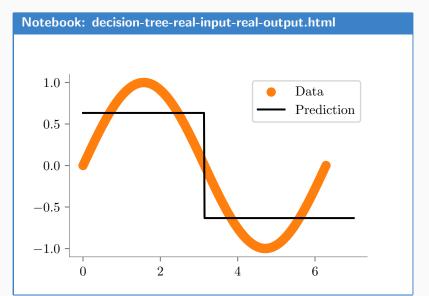
Dataset of Y = $\sin(X)$, $0 \le X \le 7$ with 10,000 points



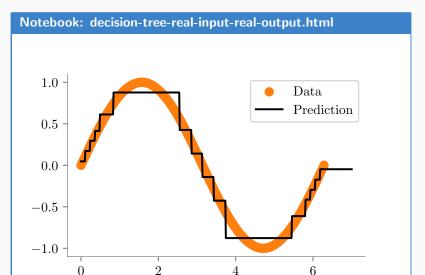
Regression tree of depth 1



Decision Boundary



Regression tree with no depth limit is too big to fit in a slide. It has of depth 4. The decision boundaries are in figure below.



• Interpretability an important goal

- Interpretability an important goal
- Decision trees: well known interpretable models

- Interpretability an important goal
- Decision trees: well known interpretable models
- Learning optimal tree is hard

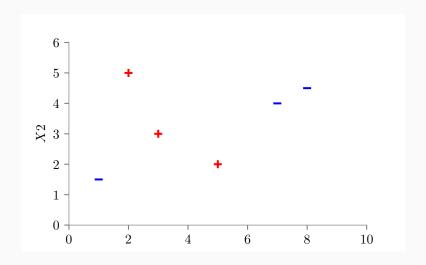
- Interpretability an important goal
- Decision trees: well known interpretable models
- Learning optimal tree is hard
- Greedy approach:

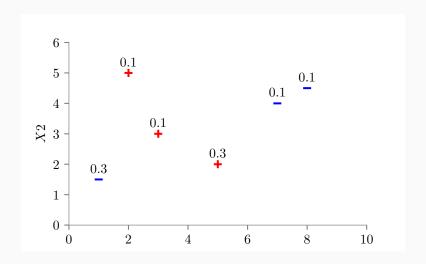
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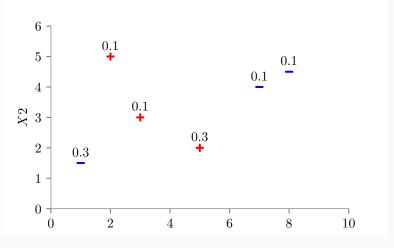
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 - Empirically not as powerful as other methods







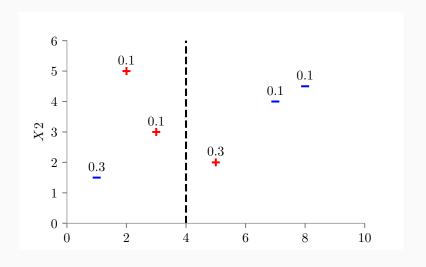
$$0 \frac{1}{0} \frac{1}{2} \frac{1}{4} \frac{1}{6} \frac{1}{8} \frac{1}{10}$$

$$= -P(+) \log_2 P(+) - P(-) \log_2 P(-)$$

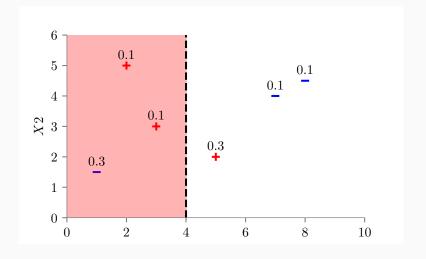
 $P(+) = \frac{0.1 + 0.1 + 0.3}{1} = 0.5, \quad P(-) = \frac{0.3 + 0.1 + 0.1}{1} = 0.5$

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Weighted Entropy

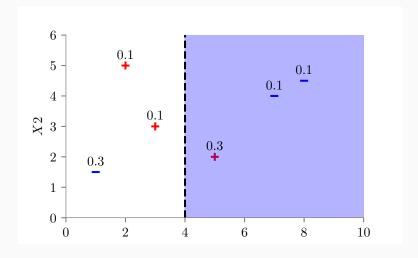


Candidate Line: $X1 = 4(X1^*)$



Entropy of $X1 \leq X1^* = E_{S(X1 < X1^*)}$

$$P(+) = \frac{0.1 + 0.1}{0.1 + 0.1 + 0.3} = \frac{2}{5}$$



Entropy of $X_1>X_1^*=E_{\mathcal{S}(X_1>X_1^*)}$

$$P(+) = -$$

$$\begin{bmatrix} 6 \\ 5 \\ 4 \\ 4 \\ 2 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 0.1 \\ 0.1 \\ 0.3 \\ 4 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 0.3 \\ 4 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 0.3 \\ 4 \\ 0 \end{bmatrix}$$

$$IG(X_1 = X_1^*) = E_S - \frac{0.5}{1} \cdot E_{S(X_1 < X_1^*)} - \frac{0.5}{1} \cdot E_{S(X_1 > X_1^*)}$$